**Lecture 16: Resource estimates**
Reading: Reiher et al PNAS (2017).

# 1 Introduction

After all the algorithms we have discussed, it is worthwhile to think about the quantum resources required to solve problems of physical interest. A few groups have done that, with one example being the Reiher paper referenced above. We will go through this paper to get a sense of the order of magnitude of gate counts required for a standard eigenvalue estimation problem, assuming Trotterization of the propagator.

A few notes before we begin. First, Li et al argue that the active space chosen in this paper is not correct [1]: "the active space does not actually contain the representative features of the electronic structure of the low-energy states of FeMoco that make its classical (and potentially quantum) simulation difficult." In fact, Li et al show that the problem treated in the Reiher paper is classically tractable. However, Li et al also state that the resource estimates are likely not substantially affected by this issue and so we proceed. Second, new algorithms have led to decreased gate counts by about an order of magnitude, for instance in Ref. [2]. However, these decreases don't affect the final conclusion that phase estimation for realistic electronic structure Hamiltonians will not be feasible for quite some time, and so we proceed with the Reiher paper.

# 2 Flow of calculation

The goal of an electronic structure calculation on a quantum computer is to obtain the correlation energy, defined as the difference between the Hartree-Fock energy with a converged basis set and the true ground state energy. Often the calculation is performed in a restricted "active space" since certain orbitals may not be sensitive to correlation effects. The general flow of the algorithm would be to generate an active space via a HF calculation, and then implement phase estimation to obtain the correlation energy.

We take as a given that the computation needs to be implemented in a fault-tolerant way with error correction due to the gate depth required, and so we need a brief discussion of error correction. Quantum error correction (QEC) protects a discrete set of gates against errors, and this discrete set can be used to implement any other gate. First, exponentials are decomposed into single qubit rotations and Clifford gates; the latter gates can implemented fault-tolerantly in an error correction scheme known as a surface code. However, to approximate arbitrary rotations we need one non-Clifford gate such as a T gates. Implementing such a gate requires a scheme known as "magic state distillation", in which noisy quantum states are manipulated to produce an accurate magic state and a T gate is teleported into the system register. The upshot is that implementing T gates requires substantial resources and is thus expensive. Groups of qubits known as T factories are required to implement these gates.

# 3 Gate count estimates

We now proceed to the estimates for gate counts. In the paper, various scenarios and assumptions are considered; a simplified description is presented below:

1. Logical T gates take 10 or 100 ns
2. An estimate of the ground state wavefunction is available (to make phase estimation yield the ground state energy)

3. Clifford gates take negligible time relative to the T gates

4. Various error rates are assumed, including $10^{-3}$, 100 ns duration for near-term superconducting qubits, and $10^{-6}$ and 10 ns for aspirational hardware.

5. Implementation of the algorithm occurs in series (all rotations one after another), nesting (disjoint spins are done in parallel), and programmable ancilla rotations (PAR, rotations are precomputed in parallel factories and teleported in)

First, the overhead of error correction is neglected. To obtain quantitative accuracy (defined as energy accuracy to within 0.1 mHa), the serial scheme requires $O(10^{15}$ gates, 111 logical qubits, and 3+ years to complete. Pretty expensive! For the nesting scheme, the same order of gates are required, 135 logical qubits, and 5 months. For qualitative accuracy, these numbers reduce to $O(10^{14})$ gates, 4 months for serial, and 14 days for nesting. Clearly we need many orders of magnitude improvement in coherence time or, more realistically, error correction before such calculations are feasible. The estimation also highlights the importance of having fast gates - for some architectures that support gates at kHz rates like ion traps, the number of gates presented above are simply not possible.

Now consider the overhead required for error correction. Say we have $10^{-3}$ error rate, serial execution. We will need $\sim 150,000$ physical qubits per logical qubit, 202 T factories with $\sim 10^6$ physical qubits per factory. The total number of physical qubits is $\sim 200 \times 10^6$ - a lot! The situation of course improves with topological qubits with $O(10^{-9})$ error rate, but first we need topological qubits.

A more recent estimate of gate counts was given in [2] using a different algorithm. There it was concluded that similar energy estimations require on the order of 350 Megaqubitdays - or 1 million physical qubits for 350 days! Such a resource requirement is less than that presented in the Reiher paper but still substantial.

The generic conclusions we can draw:

1. Good approximation schemes and algorithmic improvements are still needed to make calculations give useful results in a reasonable amount of time

2. Any useful calculation for ground state energies (e.g. one that can be performed on a classically intractable instance) using phase estimation will certainly require error correction at a large scale.

## References

[1] Z. Li, J. Li, N. S. Dattani, C. J. Umrigar, and G. K.-L. Chan, "The electronic complexity of the ground-state of the femo cofactor of nitrogenase as relevant to quantum simulations", The Journal of Chemical Physics **150**, 024302 (2019).

[2] D. W. Berry, C. Gidney, M. Motta, J. R. McClean, and R. Babbush, "Qubitization of arbitrary basis quantum chemistry by low rank factorization", arXiv (2019).